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Unifying the Mechanics of Continua, Cracks, and Particles

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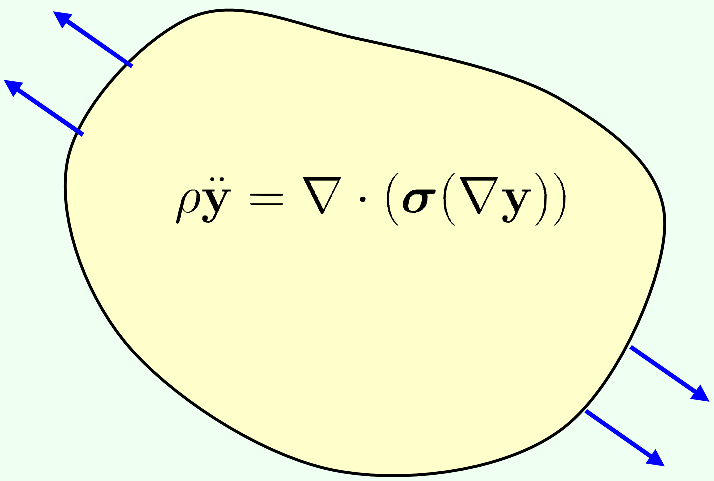
Outline

- Limitations of the classical theory of solid mechanics
- Peridynamic theory: how it works
  - Numerical examples
- Length scales
- Relation between peridynamic and classical theories
- Mathematical consistency and numerical convergence

Particles vs. continua: the issue

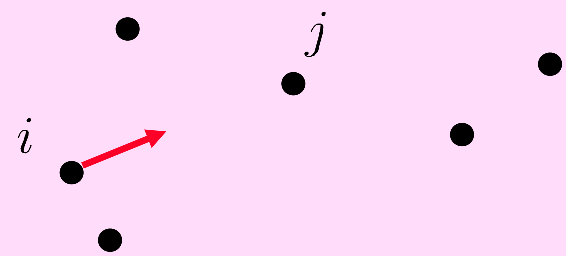
• Standard continuum mechanics is incompatible with the essential physical nature of particles.



$$\rho\ddot{\mathbf{y}} = \nabla\cdot(\boldsymbol{\sigma}(\nabla\mathbf{y}))$$

Continuous body:

- Local interactions
- Contact forces
- Continuous distribution of mass
- Smooth deformation



$$M_i\ddot{\mathbf{y}}_i = \sum_j \mathbf{F}_{ij}(\mathbf{y}_j - \mathbf{y}_i)$$

Particles:

- Nonlocal interactions
- Long-range forces
- Discontinuous distribution of mass

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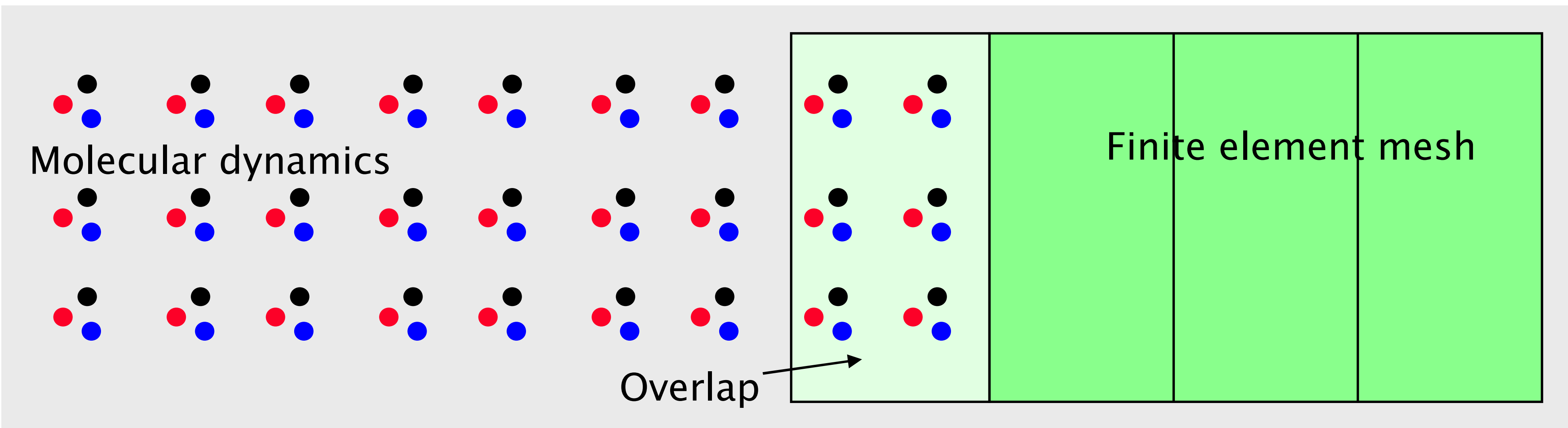
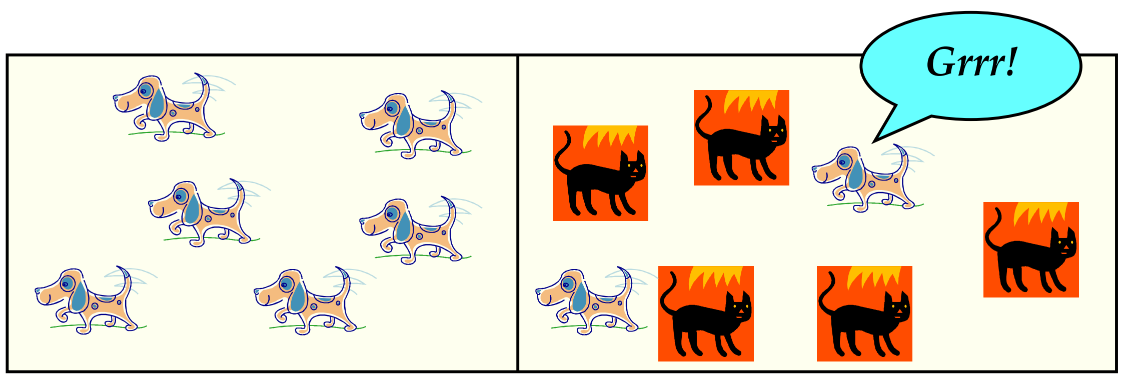
Particles vs. continua:
Why this issue is important

- Current atomistic-to-continuum coupling methods require connecting fields that have dissimilar mathematical properties.





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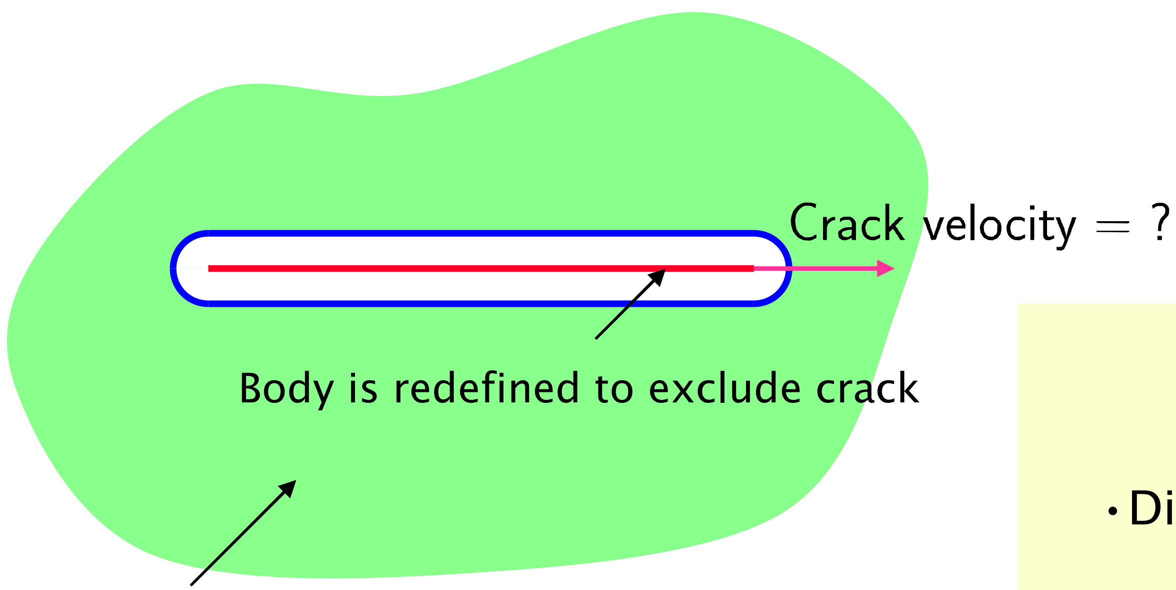
Cracks: the issue

- Standard continuum mechanics is incompatible with the essential physical nature cracks.
  - Can't apply the PDEs directly on a crack.
  - Typical approaches require some fix at the discretized level.



Cracks:

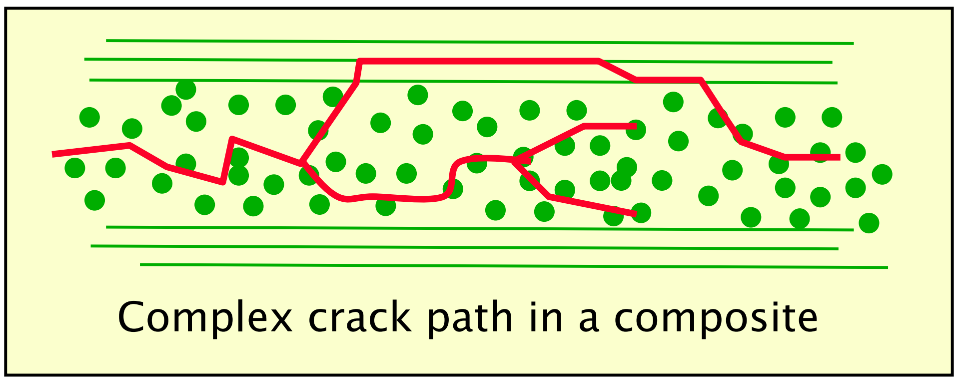
- Nonlocal interactions
- Discontinuous deformation

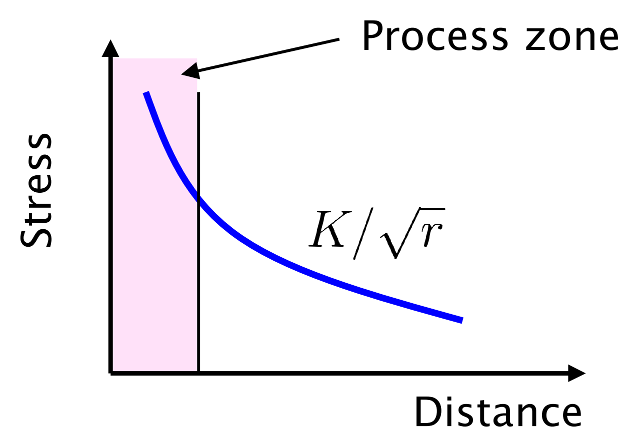
$$\rho\ddot{\mathbf{y}} = \nabla\cdot(\boldsymbol{\sigma}(\nabla\mathbf{y})) + \mathbf{b}$$

applies everywhere except the crack.

Cracks:
Why this is important

- Kinetic relations of fracture mechanics can only be determined in idealized cases.
  - FM assumes geometric length scale >> process zone.





The reality of fracture may be too complex to represent in the form

$$\dot{a} = f(K)$$

What the peridynamic theory seeks to provide

- To predict the mechanics of continuous and discontinuous media with mathematical consistency.
  - Everything should emerge from the same continuum model.

- Why do this?
  - Hope to achieve a more general, accurate, elegant, flexible means of modeling A-to-C coupling and fracture in complex media.

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Strategy of the peridynamic theory

Replace the standard PDEs with integral equations.

- The integral equations involve interaction between points separated by finite distances (nonlocality).
- The integral equations are not derivable from the PDEs.

PERGAMON

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Reformulation of elasticity theory for discontinuities and long-range forces

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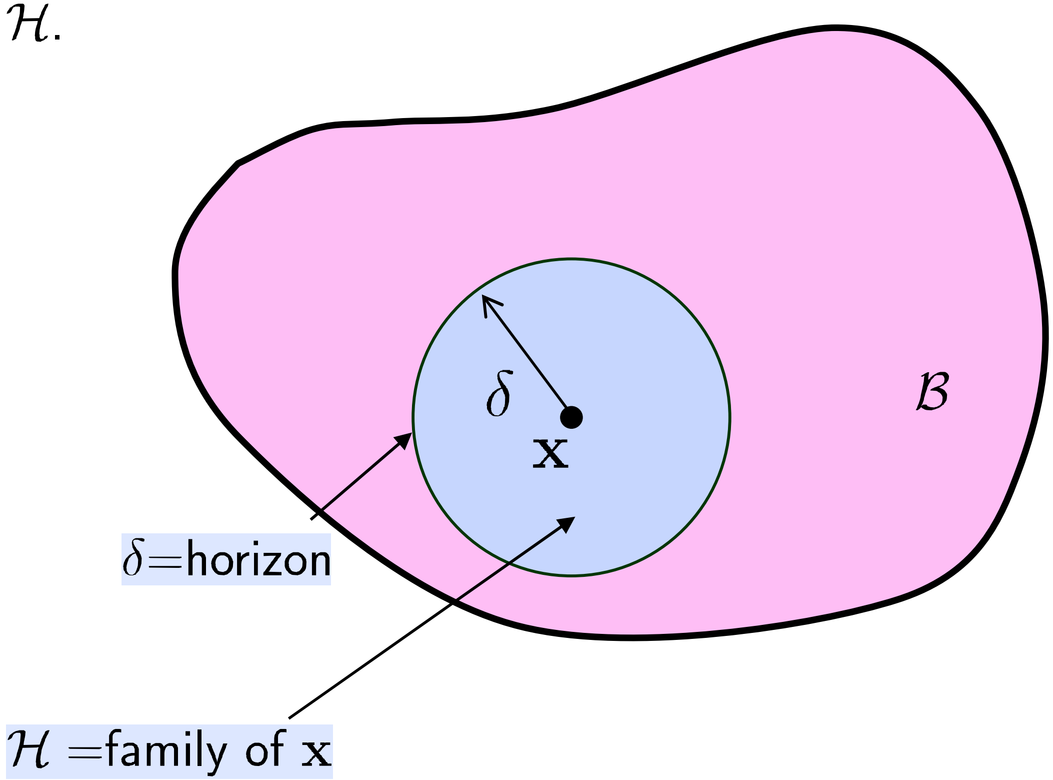
Peridynamics basics: Horizon and family

- Any point $\mathbf{x}$ interacts directly with other points within a finite distance δ called the "horizon."
- The material within a distance δ of $\mathbf{x}$ is called the "family" of $\mathbf{x}$, $\mathcal{H}$.



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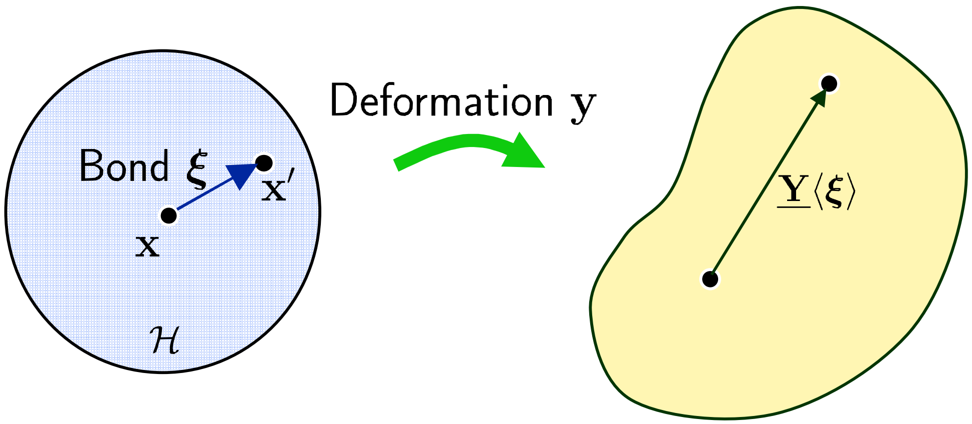
Starting point for peridynamics

Strain energy at $\mathbf{x}$ depends collectively on the deformation of the family of $\mathbf{x}$.



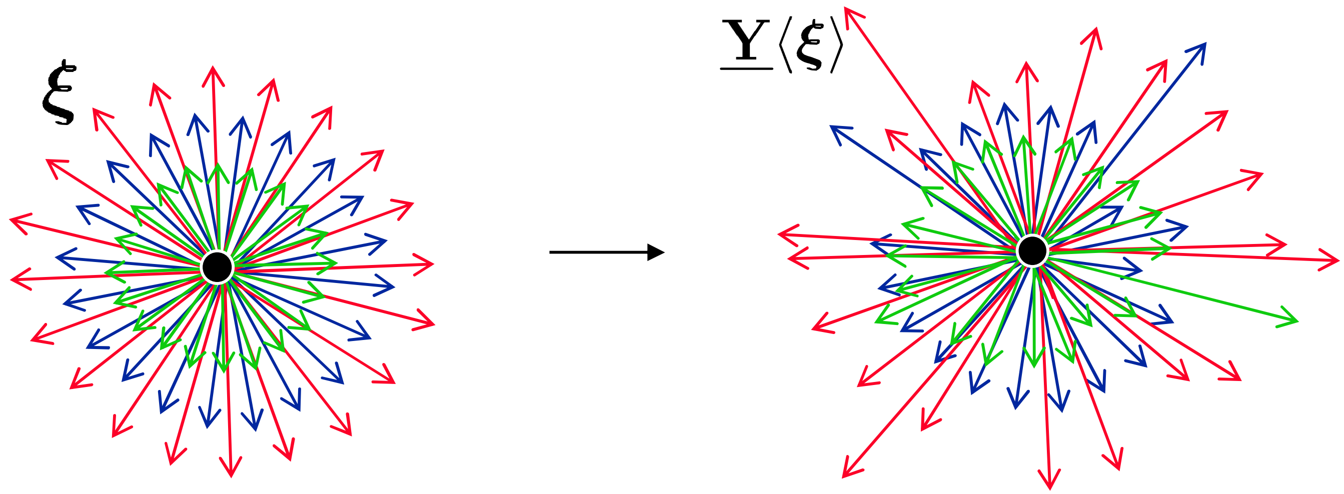
Undeformed family of $\mathbf{x}$

Deformed family of $\mathbf{x}$

Standard:	Peridynamic:
$W\left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)$	$W(\underline{\mathbf{Y}})$

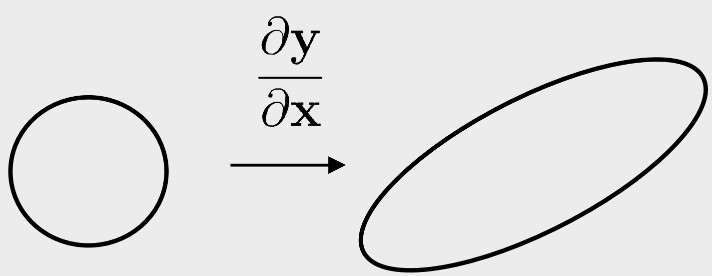
The deformation state is the function that maps each bond $\boldsymbol{\xi}$ into its deformed image $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$.

Deformation states can contain a lot of kinematical complexity



Undeformed bonds connected to $\mathbf{x}$

Deformed bonds connected to $\mathbf{x}$



Compare this with standard theory in which small spheres are mapped into ellipsoids

Force state is the work conjugate to the deformation state

- Suppose we perturb the deformed bond $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$ by a virtual displacement $\boldsymbol{\epsilon}$. The resulting change in $W(\mathbf{x})$ is

$$\Delta W = \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \cdot \boldsymbol{\epsilon}$$

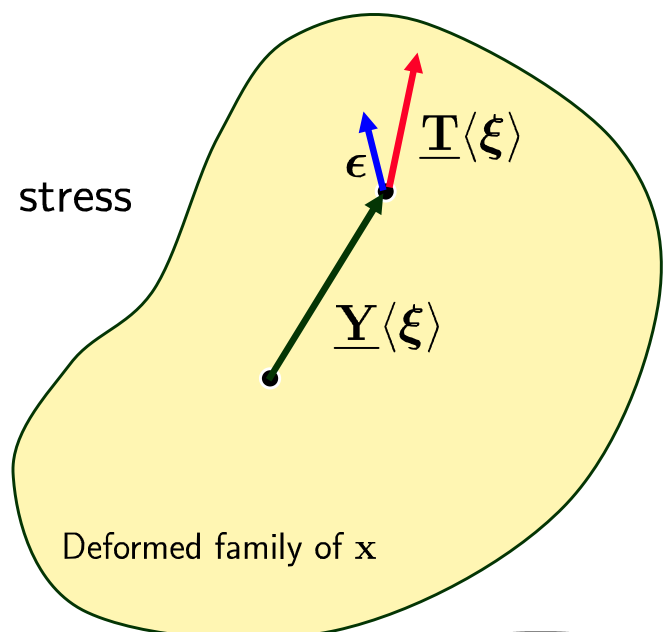
  where $\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle$ is a vector.

- The "force state" $\underline{\mathbf{T}}$ is the work conjugate to $\underline{\mathbf{Y}}$:

$$\dot{W} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} = \int_{\mathcal{H}} \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \cdot \dot{\underline{\mathbf{Y}}}\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}}$$

- $\underline{\mathbf{T}}$ is the Frechet derivative of $W(\underline{\mathbf{Y}})$ – analogous to a stress tensor.

Displace just one bond $\boldsymbol{\xi}$



Peridynamic equilibrium equation

- Total potential energy in $\mathcal{B}$:

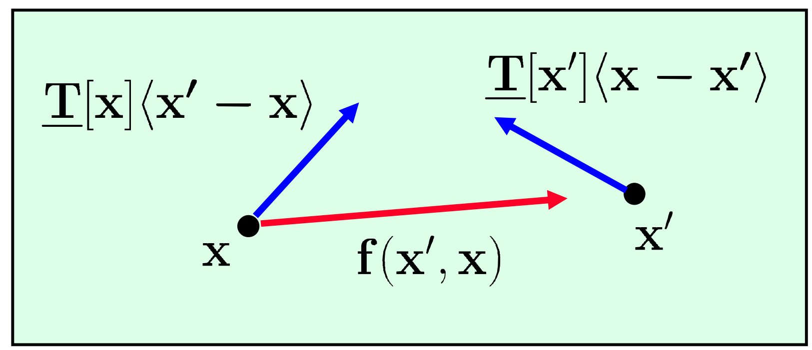
$$\Phi_{\mathbf{y}} = \int_{\mathcal{B}} (W(\underline{\mathbf{Y}}) - \mathbf{b} \cdot \mathbf{y})\, dV_{\mathbf{x}}$$

- Take first variation. Euler-Lagrange equation is

$$\int_{\mathcal{H}} \left(\underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}.$$

- Write this in terms of the "bond force" :

$$\int_{\mathcal{H}} \mathbf{f}(\mathbf{x}', \mathbf{x})\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}.$$



- where the bond force is defined by

$$\mathbf{f}(\mathbf{x}', \mathbf{x}) = \underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle$$

Peridynamic equation of motion

- Equilibrium equation:

$$\int_{\mathcal{H}} \mathbf{f}(\mathbf{x}', \mathbf{x}) \, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}.$$

- where

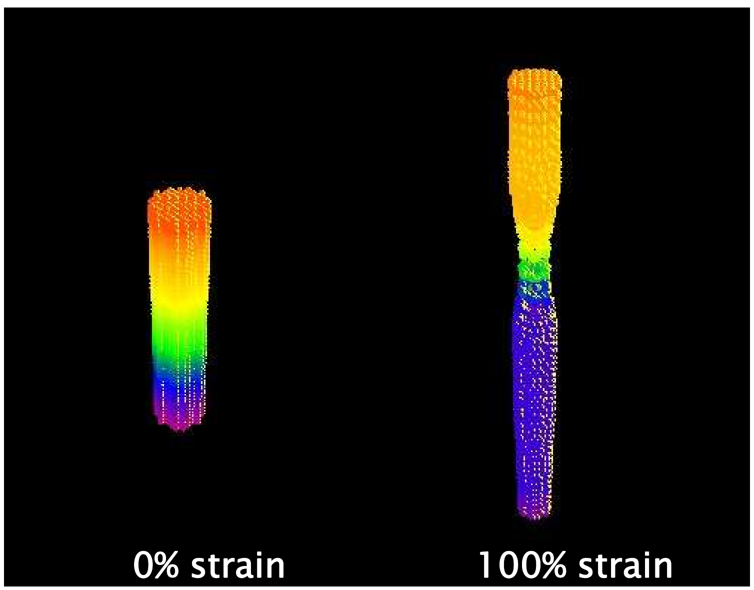
$$\mathbf{f}(\mathbf{x}', \mathbf{x}) = \underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle$$

- Now use d'Alembert's principle to get the equation of motion:

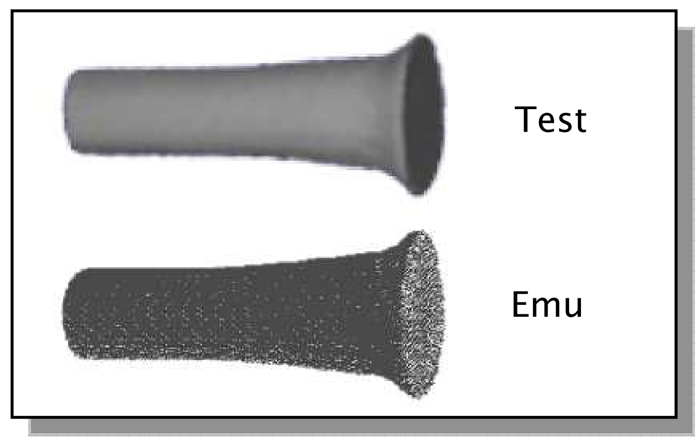
$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x}, t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}', \mathbf{x}, t) \, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

Continuum material models

- Any material model in the standard theory can be adapted to the peridynamic theory.
- Example: EMU simulation with large-deformation, strain-hardening, rate-dependent material model.
  - Material model implementation by J. Foster.



Necking under tension



Taylor impact test

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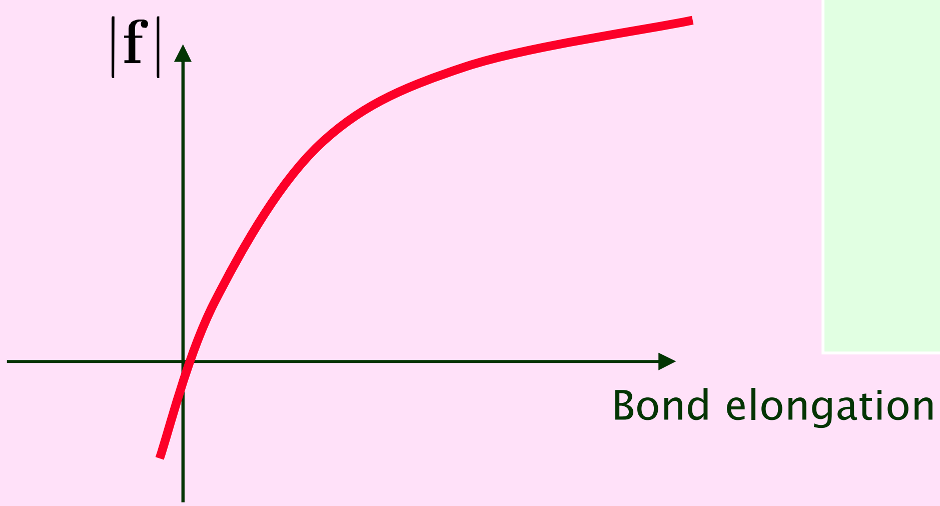
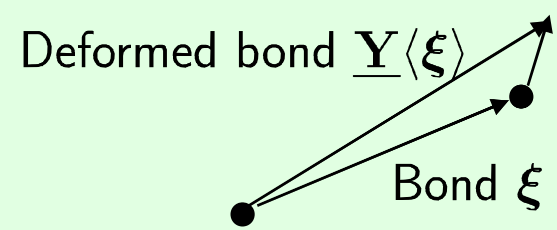
Continuum material models, ctd.

- The simplest assumption is that all the bonds are independent.
- Equation of motion simplifies to

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{y}(\mathbf{x}',t) - \mathbf{y}(\mathbf{x},t), \mathbf{x}', \mathbf{x})\, dV_{\mathbf{x}} + \mathbf{b}(\mathbf{x},t),$$

- The body is in effect a network of nonlinear springs.





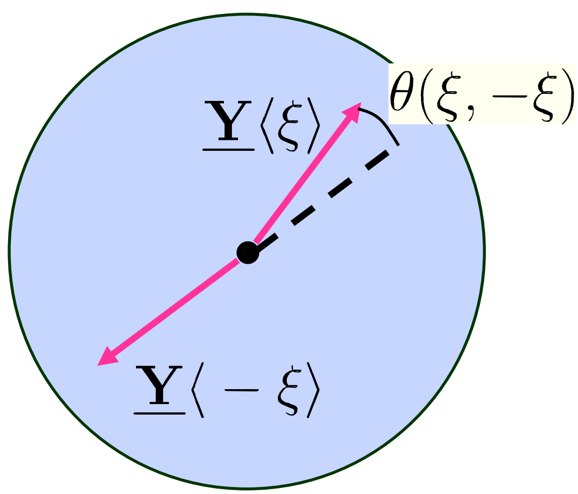
Bond elongation $= |\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}|$

Continuum material models, ctd.

- Can also have materials that have no analogue in the standard theory:
- Example: A material that responds to angle changes between pairs of bonds:

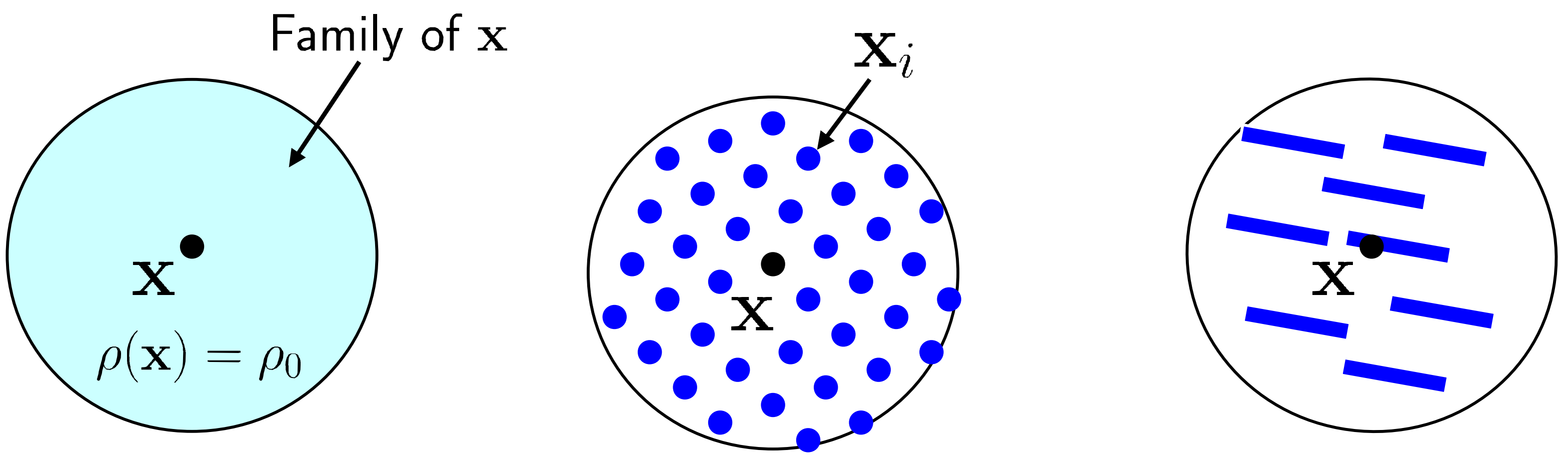
$$W = \frac{1}{2} \int \left(\pi - \theta(\xi, -\xi)\right)^2 \, dV_\xi$$

where $\theta(\xi, -\xi)$ is the deformed angle between bonds ξ and $-\xi$.



Peridynamic model of a system of discrete particles

- The family of $\mathbf{x}$ could be either continuous or a collection of point masses or other objects.



$$\rho(\mathbf{x}) = m \sum_i \Delta(\mathbf{x} - \mathbf{x}_i)$$

Δ = 3D Dirac delta function

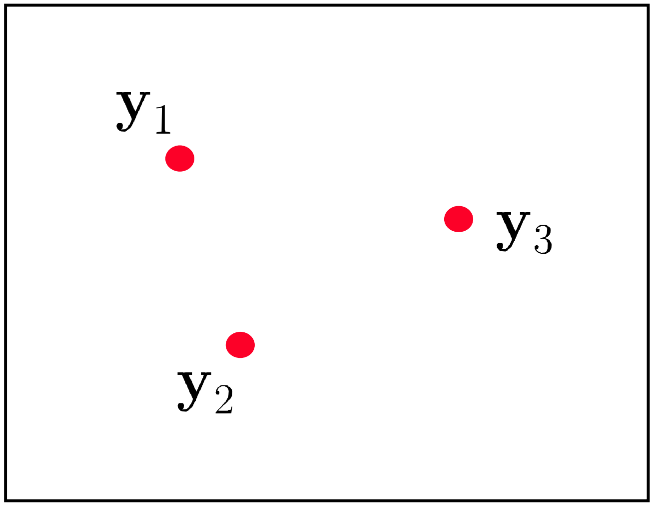
Discrete particles and PD states

- Consider a set of atoms that interact through an $N-$body potential:

$$U(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N),$$

$\mathbf{y}_1, \dots, \mathbf{y}_N =$ deformed positions, $\mathbf{x}_1, \dots, \mathbf{x}_N =$ reference positions.

- This can be represented exactly as a peridynamic body.

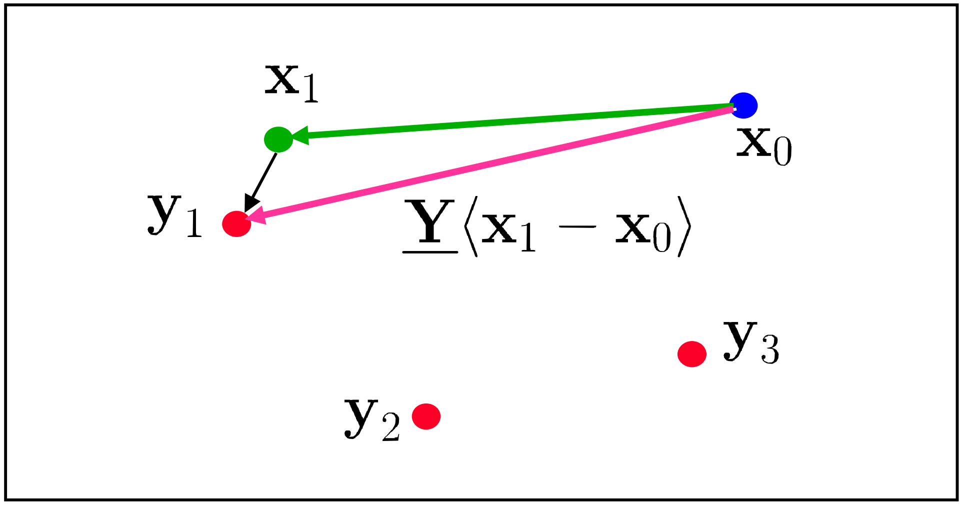


Discrete particles and PD states, ctd.

Define a peridynamic body by:

$$\hat{W}(\underline{\mathbf{Y}}, \mathbf{x}) = \Delta(\mathbf{x}-\mathbf{x}_0)U(\underline{\mathbf{Y}}\langle\mathbf{x}_1-\mathbf{x}_0\rangle, \underline{\mathbf{Y}}\langle\mathbf{x}_2-\mathbf{x}_0\rangle, \dots, \underline{\mathbf{Y}}\langle\mathbf{x}_N-\mathbf{x}_0\rangle),$$

$$\rho(\mathbf{x}) = \sum_i \Delta(\mathbf{x}-\mathbf{x}_i)M_i$$



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Discrete particles and PD states, ctd.

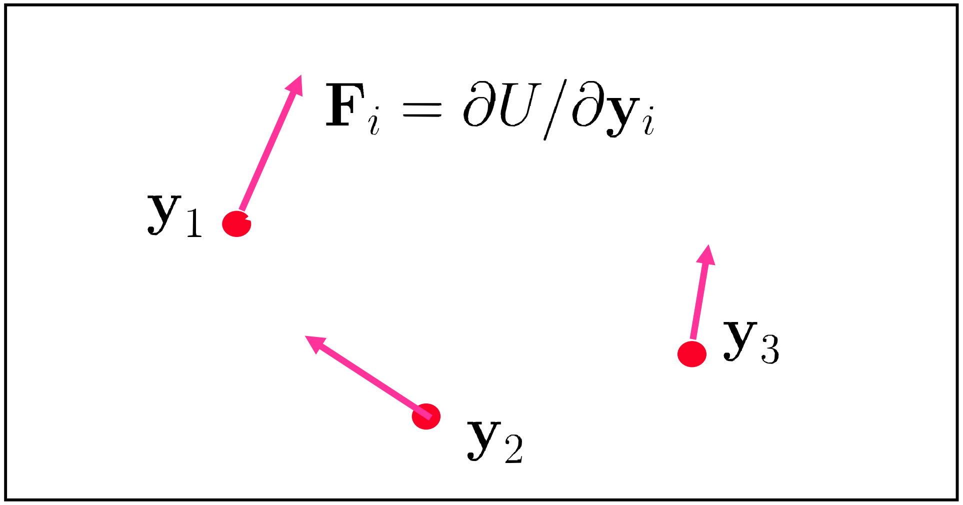
After evaluating the Frechet derivative $\underline{\mathbf{T}}$, find

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \int \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'}$$

implies

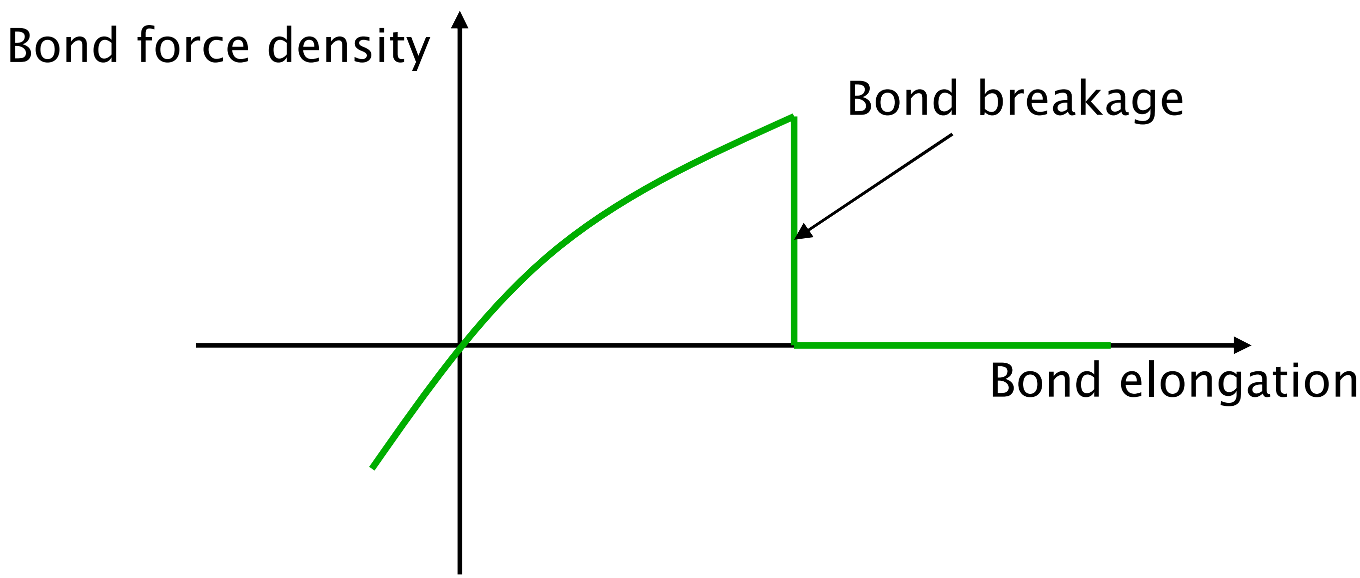
$$M_i\ddot{\mathbf{y}}(\mathbf{x}_i,t) = -\frac{\partial U}{\partial \mathbf{y}_i}, \qquad i = 1,\dots,N$$

In other words, the PD equation of motion reduces to Newton's second law.

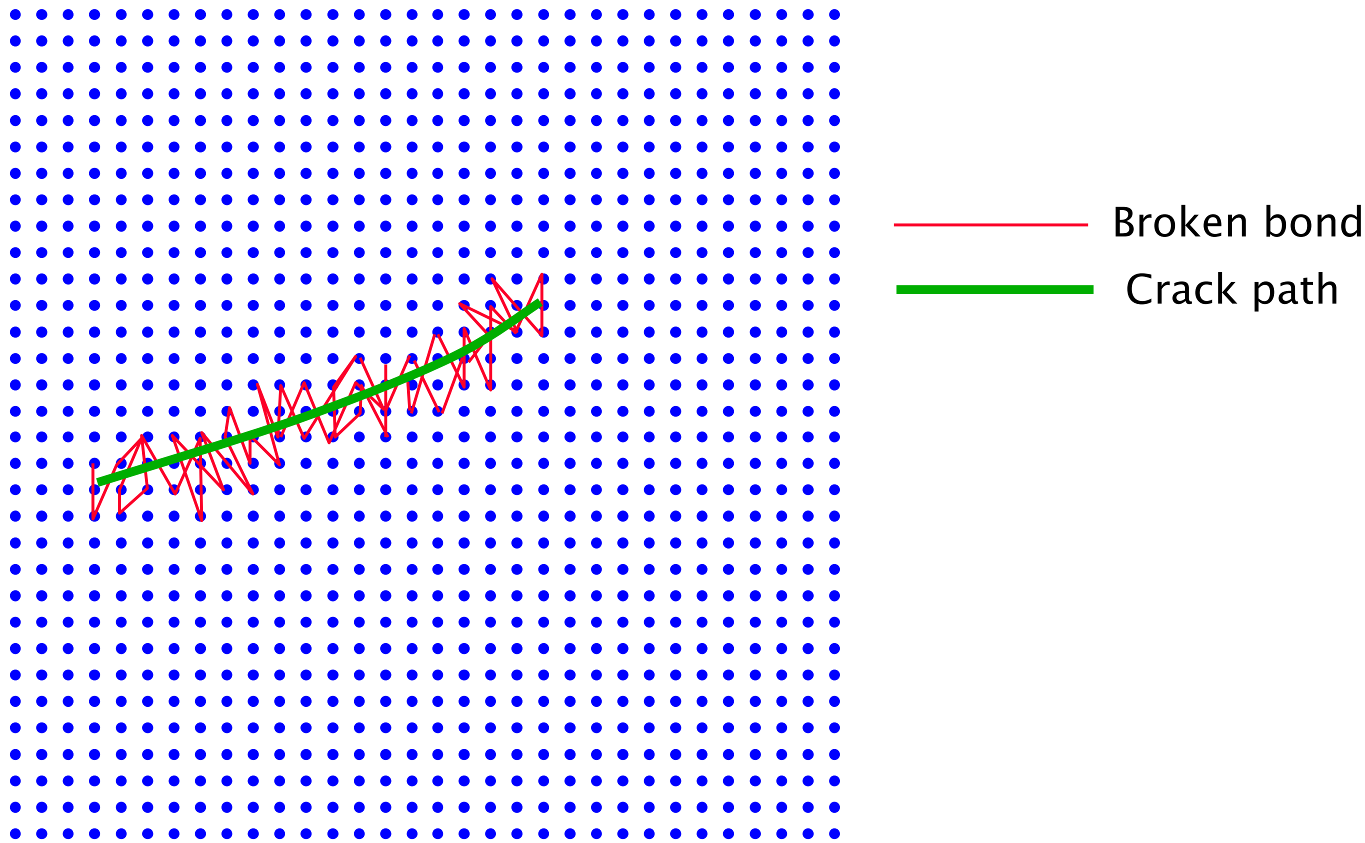


How damage and fracture are modeled

- Bonds can break irreversibly according to some criterion.
- Broken bonds carry no force.



Bond breakage forms cracks “autonomously”

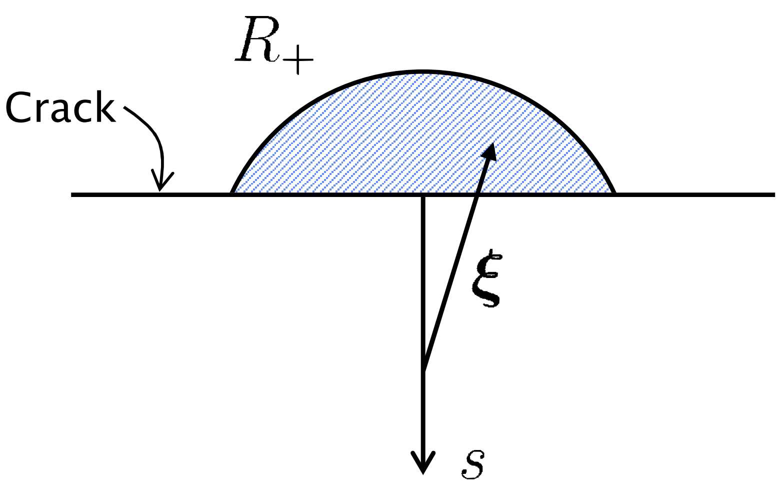


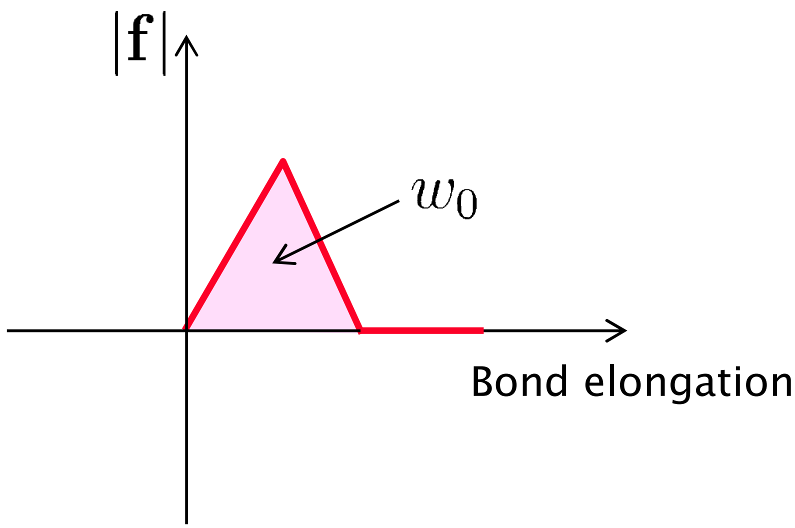
When a bond breaks, its load is shifted to its neighbors, leading to progressive failure.

Energy balance for an advancing crack

If the work required to break the bond $\boldsymbol{\xi}$ is $w_0(\boldsymbol{\xi})$, then the energy release rate is found by summing this work per unit crack area (J. Foster):

$$G = \int_0^\delta \int_{R_+} w_0(\boldsymbol{\xi})\, dV_{\boldsymbol{\xi}}\, ds$$





There is also a version of the J-integral that applies in this theory.

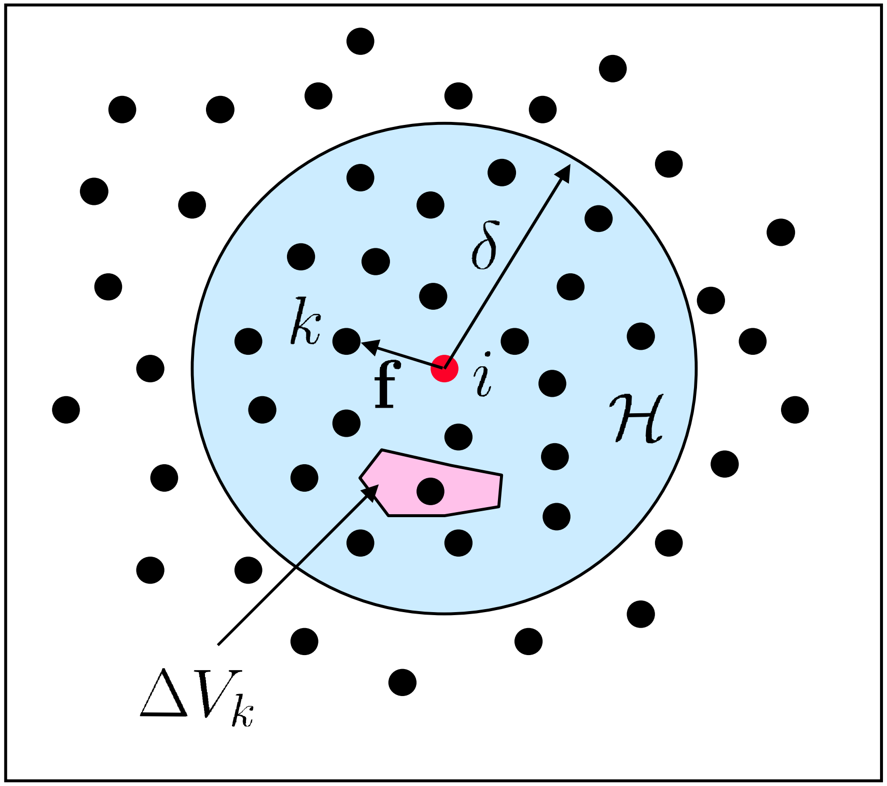
EMU numerical method

- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

$$\downarrow$$

$$\rho\ddot{\mathbf{y}}_i^n = \sum_{k\in\mathcal{H}} \mathbf{f}(\mathbf{x}_k,\mathbf{x}_i,t)\,\Delta V_k + \mathbf{b}_i^n$$



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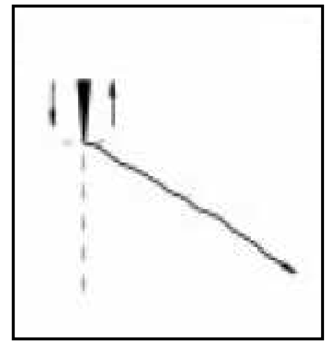
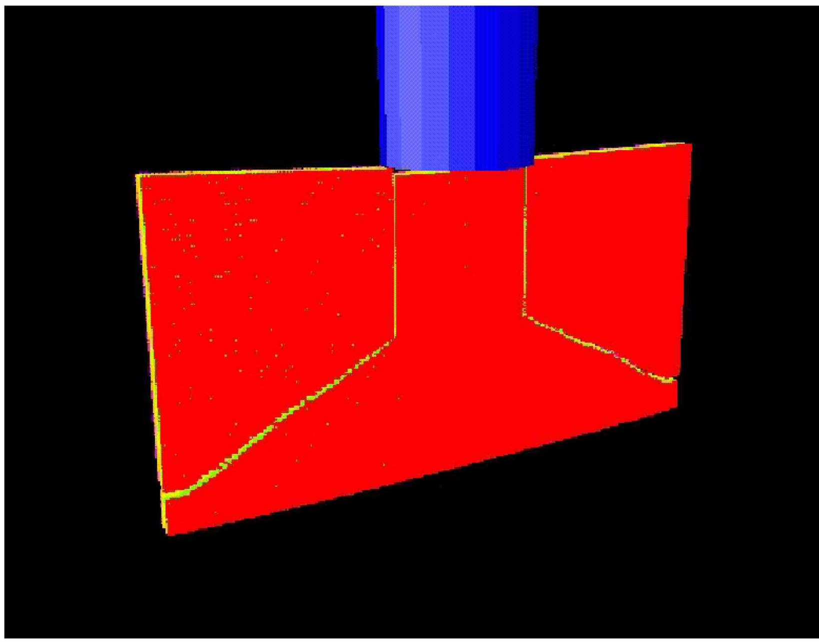
Dynamic fracture in a hard steel plate

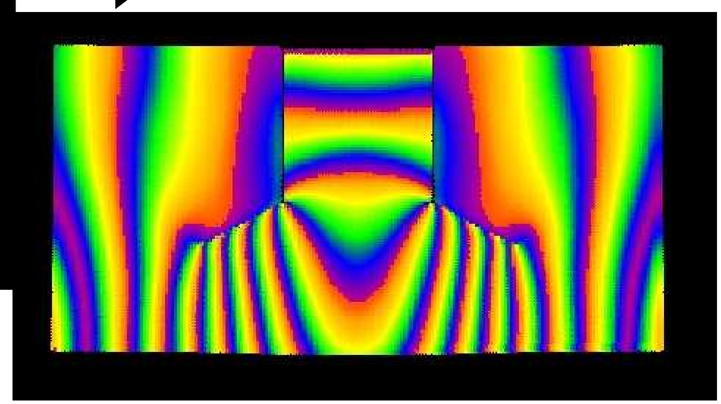
- Dynamic fracture in maraging steel (Kalthoff & Winkler, 1988)
    - Mode-II loading at notch tips results in mode-I cracks at 70deg angle.
    - 3D EMU model reproduces the crack angle.



Experiment

EMU*





S. A. Silling, Dynamic fracture modeling with a meshfree peridynamic code, in *Computational Fluid and Solid Mechanics 2003*, K.J. Bathe, ed., Elsevier, pp. 641-644.

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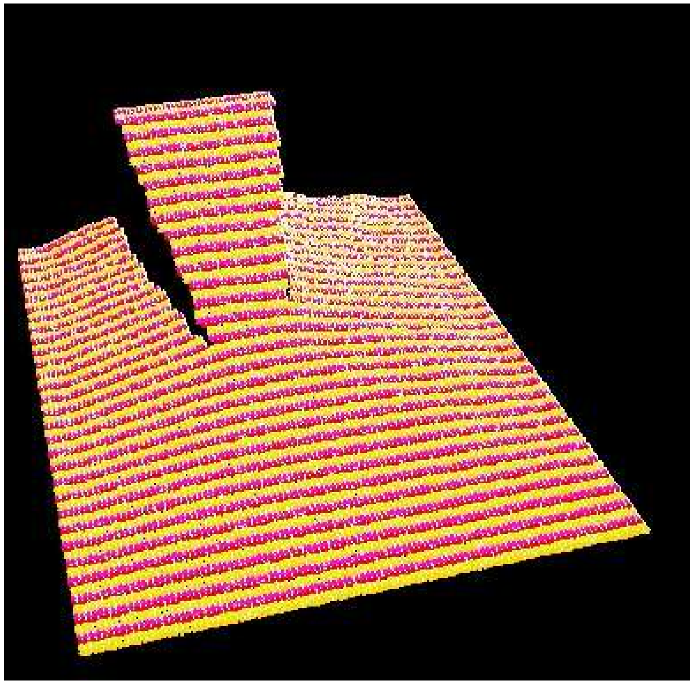
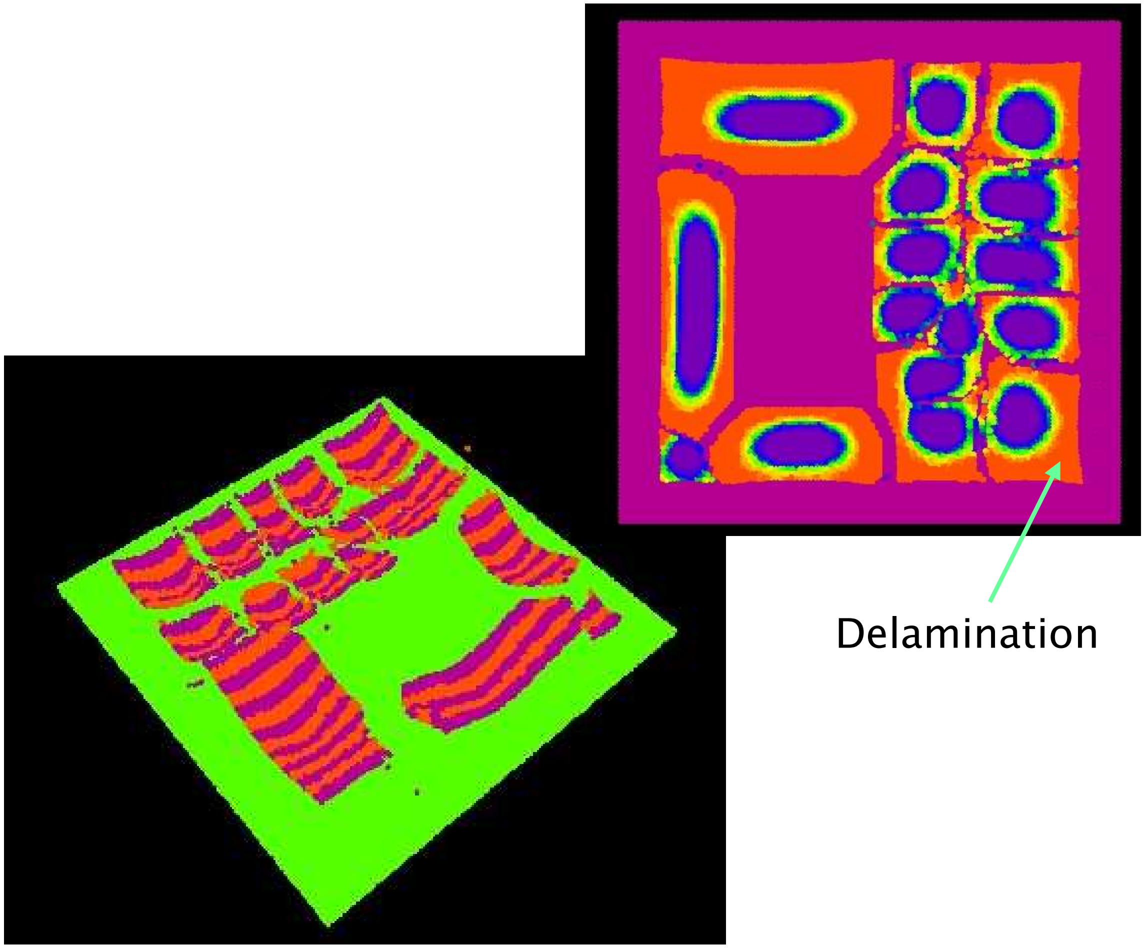
Peeling and tearing



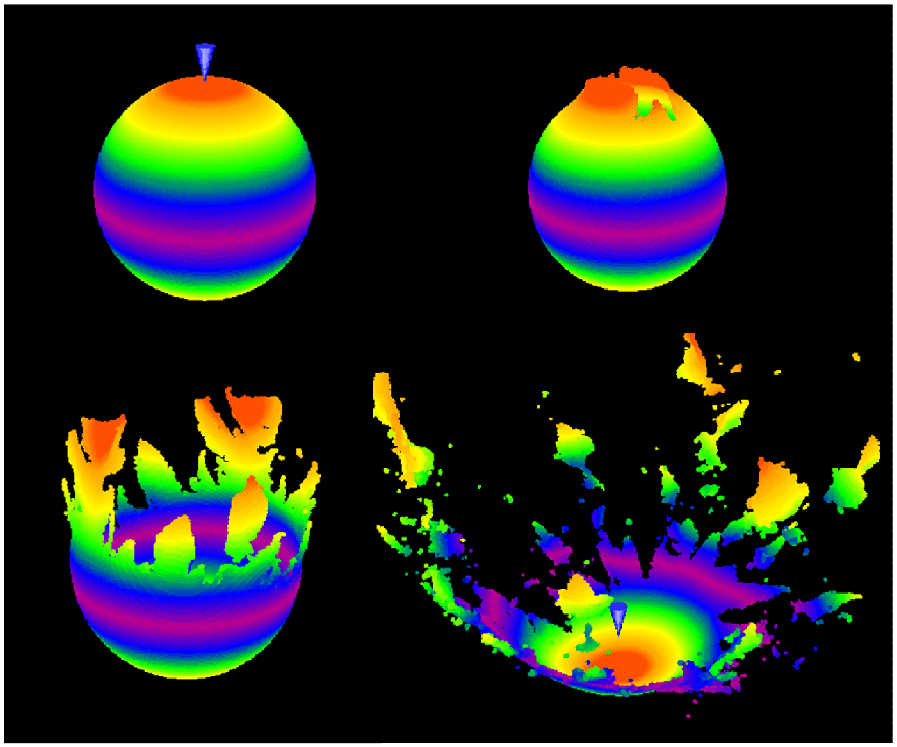
Tearing of a membrane:
Cracks are attracted to each other



Delamination

Ageing and peeling of a thin layer adhesively bonded to a substrate

Dynamic fracture in membranes



EMU model of a balloon penetrated by a fragment

Early high speed photograph by Harold Edgerton (MIT collection)
http://mit.edu/6.933/www/Fall2000/edgerton/edgerton.ppt

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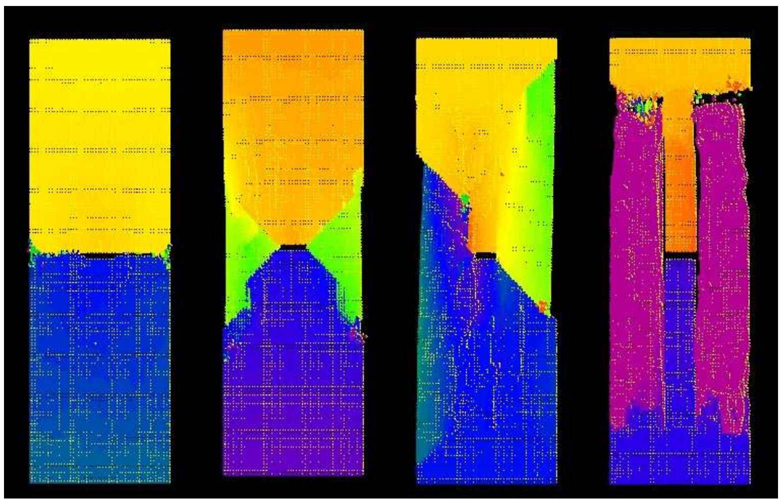
Splitting and fracture mode change in composites

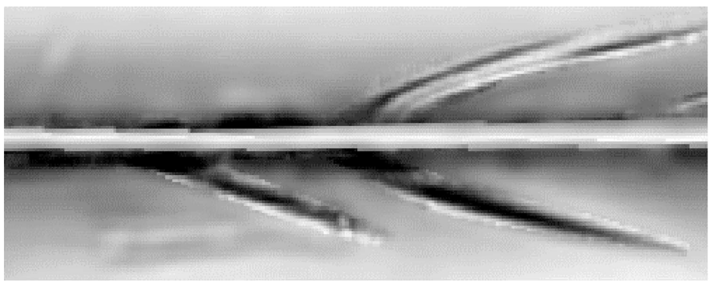
- Distribution of fiber directions between plies strongly influences the way cracks grow.



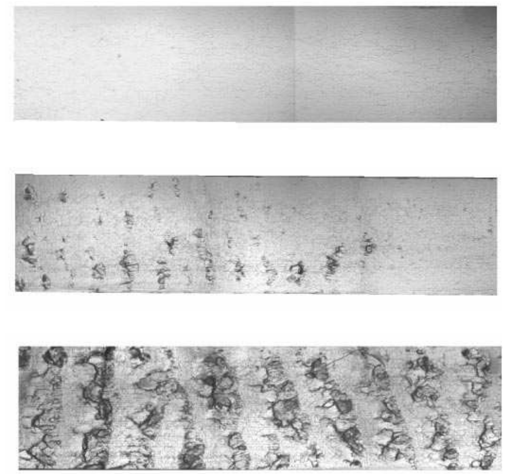
EMU simulations for different layups

Typical crack growth in a notched laminate
(photo courtesy Boeing)

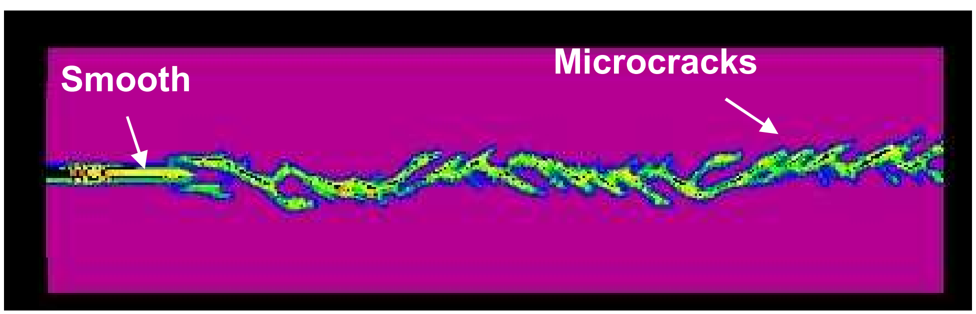
Dynamic fracture in PMMA: Damage features



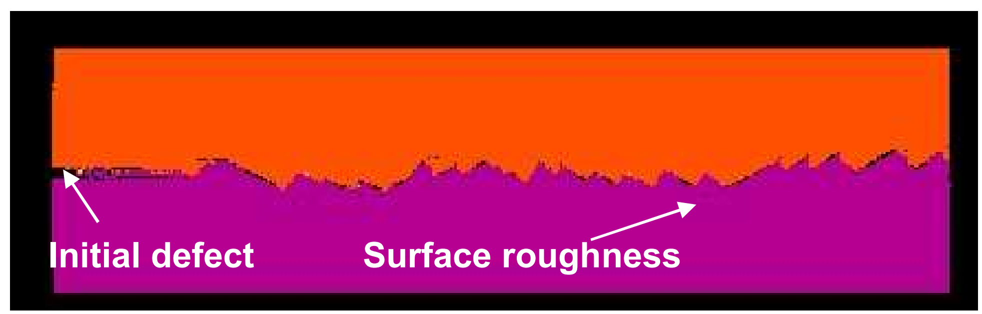
Microbranching



Mirror-mist-hackle transition*



EMU damage



EMU crack surfaces

* J. Fineberg & M. Marder, *Physics Reports* 313 (1999) 1-108

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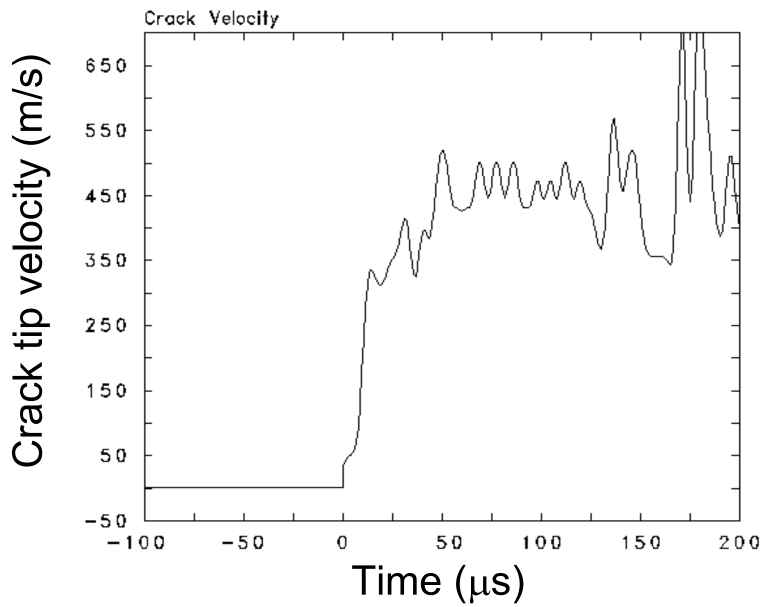
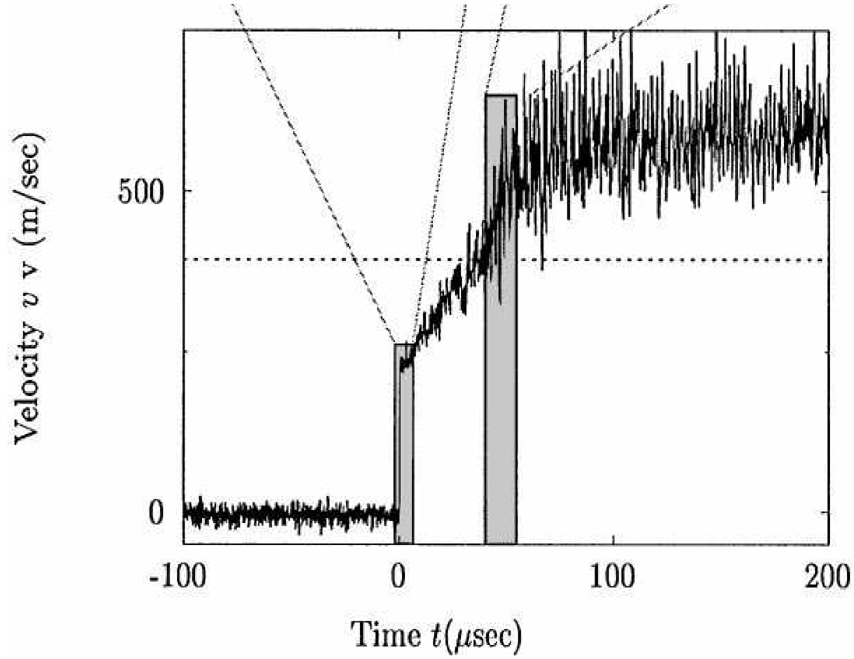
Dynamic fracture in PMMA: Crack tip velocity

- Crack velocity increases to a critical value, then oscillates.



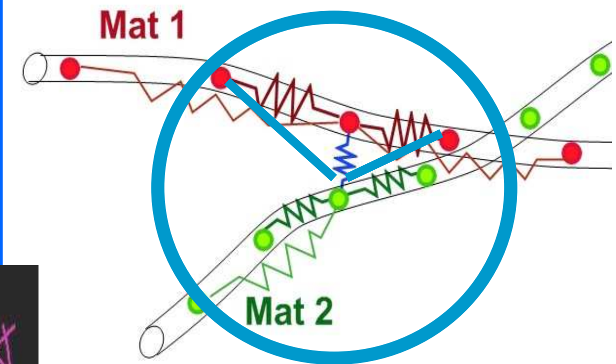
EMU



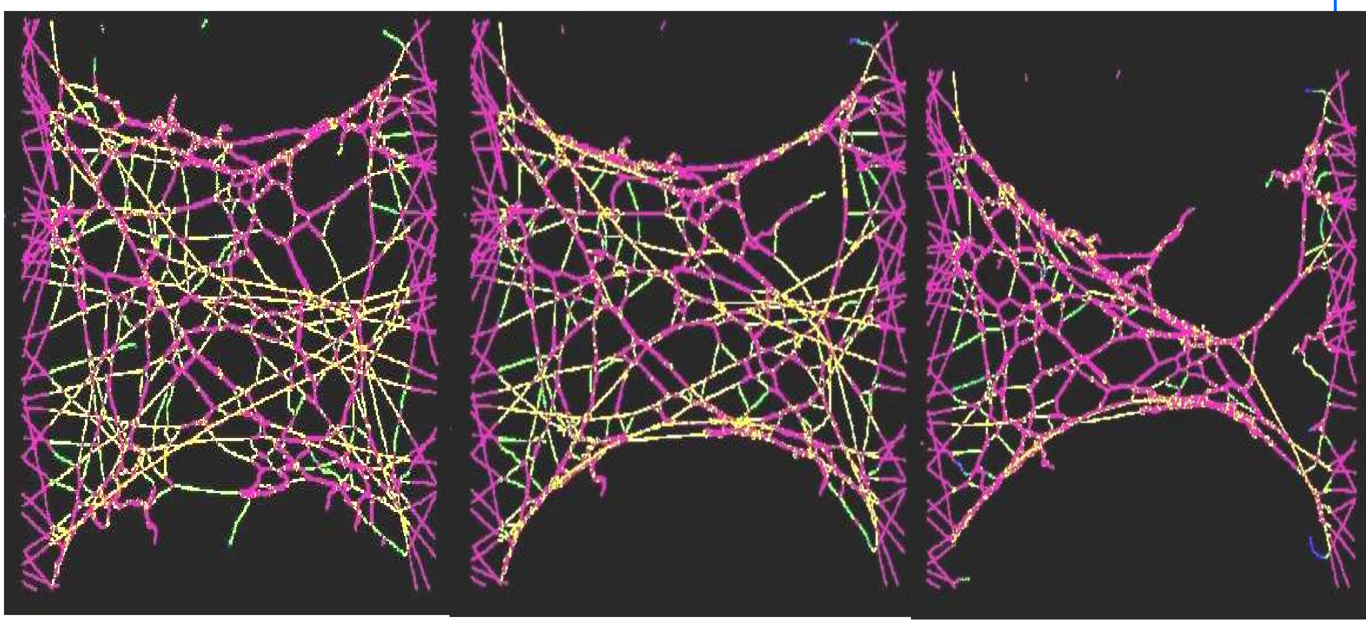
Experiment*

* J. Fineberg & M. Marder, *Physics Reports* 313 (1999) 1-108

Example of long-range forces: Nanofiber network



Nanofiber interactions due to van der Waals forces



Nanofiber membrane (F. Bobaru, Univ. of Nebraska)

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Outline

- Limitations of the classical theory of solid mechanics
- Peridynamic theory: how it works
    - Numerical examples
- Length scales
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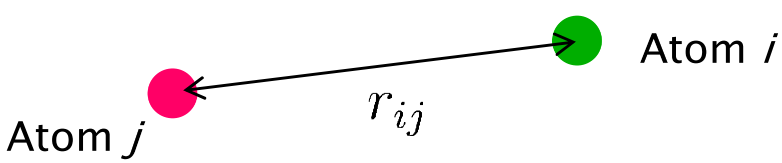
Should a continuum model have a length scale?

- Any discretization of the local PDEs is nonlocal.
  - Is there anything to be gained by moving the length scale to the continuum model?
- Many physical problems have some natural length scale.
  - Sometimes the length scale is obvious, e.g.,
    - Interatomic forces
    - Molecular dynamics cannot be done without nonlocality.



$$F_{ij} \sim \left(\frac{a}{r_{ij}}\right)^{12} - \left(\frac{a}{r_{ij}}\right)^{6}$$

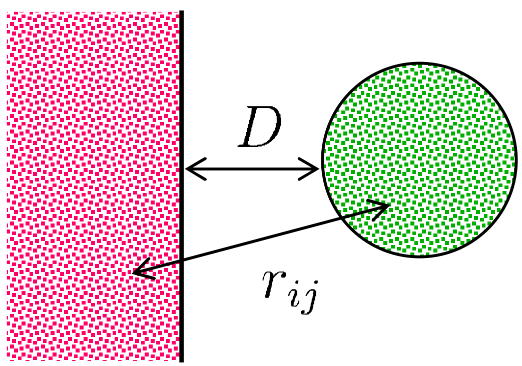
Nonlocality and length scales: surface forces

- Sometimes the length scale is a little less obvious, e.g.
  - van der Waals forces that lead to longer-range surface forces.
  - Force between a pair of atoms as they are separated:

$$F_{ij} \sim 1/r_{ij}^6$$

  - Net force between halfspace and a sphere made of many of these atoms* occurs over a much larger length scale:

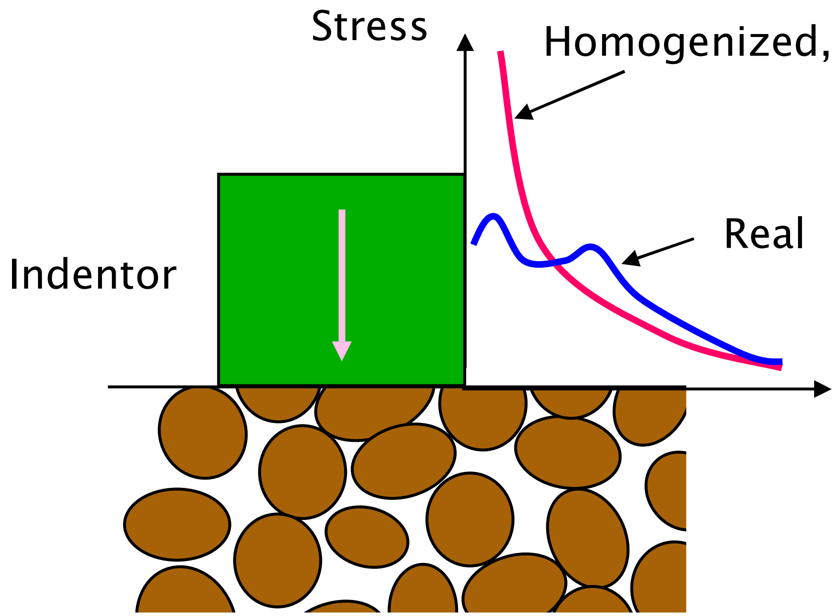
$$F_{\text{sphere}} \sim 1/D$$



See J. Israelachvili, *Intermolecular and Surfaces Forces*, pp. 177.

Nonlocality as a result of homogenization

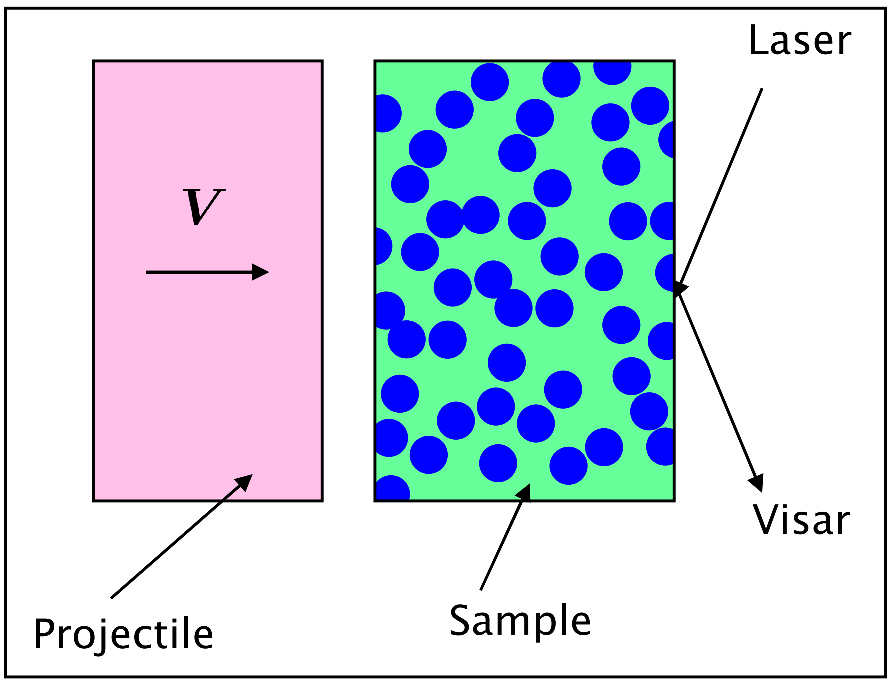
- Homogenization, neglecting the natural length scales of a system, often doesn't give good answers.

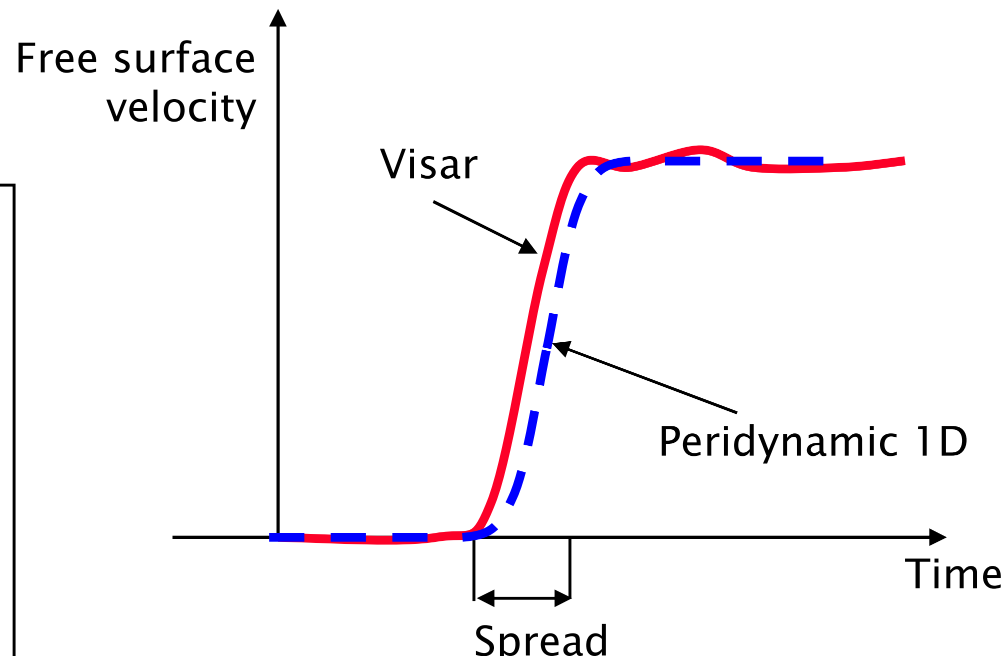


Claim: Nonlocality is an essential feature of a realistic homogenized model of a heterogeneous material.

Proposed experimental method for measuring the peridynamic horizon

- Measure how much a step wave spreads as it goes through a sample.
- Fit the horizon in a 1D peridynamic model to match the observed spread.





Local model would predict zero spread.

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Outline

- Limitations of the classical theory of solid mechanics
- Peridynamic theory: how it works
    - Numerical examples
- Length scales
- Relation between peridynamic and classical theories
- Mathematical consistency and numerical convergence

Peridynamic stress tensor

In any peridynamic body, we can define a tensor field $\boldsymbol{\nu}$ such that:

- The force per unit area at $\mathbf{x}$ through a plane with normal $\mathbf{n}$ is

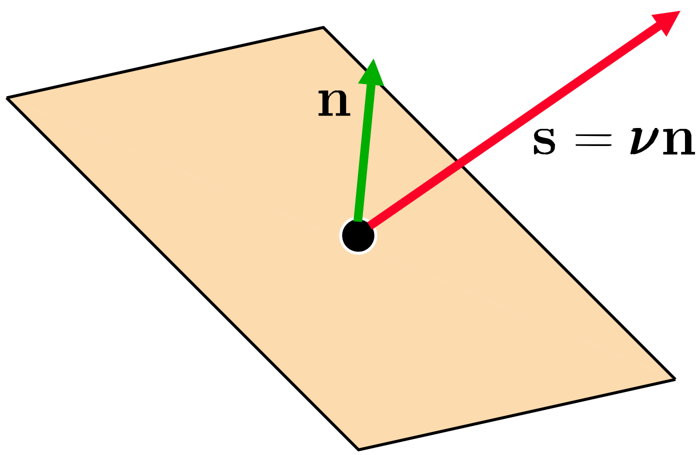
$$\mathbf{s} = \boldsymbol{\nu}(\mathbf{x})\mathbf{n}$$

- The peridynamic equation of motion can be written as

$$\rho\ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\nu} + \mathbf{b}$$

i.e.,

$$\nabla \cdot \boldsymbol{\nu}(\mathbf{x}) = \int \mathbf{f}(\mathbf{x}', \mathbf{x})\, dV_{\mathbf{x}'}$$



Convergence of peridynamics to the standard theory

Suppose the deformation is twice continuously differentiable. If the horizon is small, the deformation state is well approximated by

$$\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \approx (\nabla\mathbf{y})\boldsymbol{\xi}$$

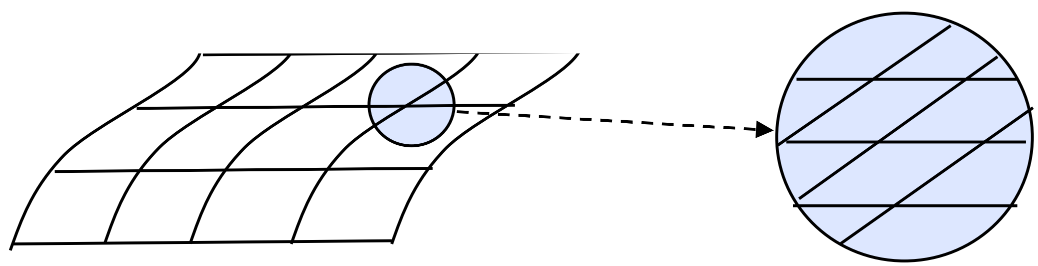
so we can write

$$W(\underline{\mathbf{Y}}) \approx W_c(\nabla\mathbf{y})$$

and it can be proven that

$$\boldsymbol{\nu} \approx \frac{\partial W_c}{\partial \nabla\mathbf{y}}$$

so $\boldsymbol{\nu}$ is basically a Piola-Kirchhoff stress tensor in a classical hyperelastic solid.



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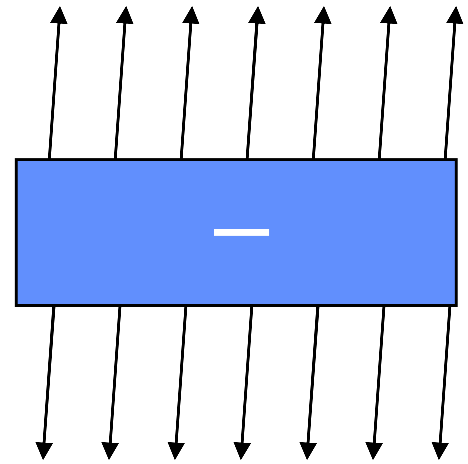
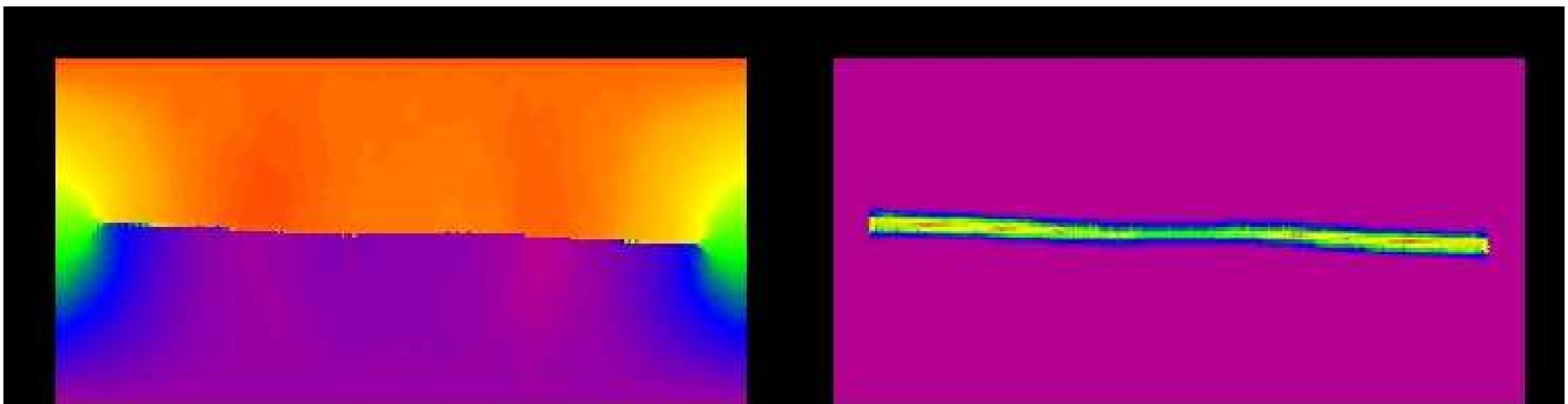
Predicted crack growth direction depends continuously on loading direction

- Plate with a pre-existing defect is subjected to prescribed boundary velocities.

- These BC correspond to mostly Mode-I loading with a little Mode-II.

$$\dot{\varepsilon} = (0.25\mathrm{s}^{-1}) \begin{bmatrix} 0 & 0.1 \\ 0 & 1 \end{bmatrix}$$





Contours of vertical displacement

Contours of damage

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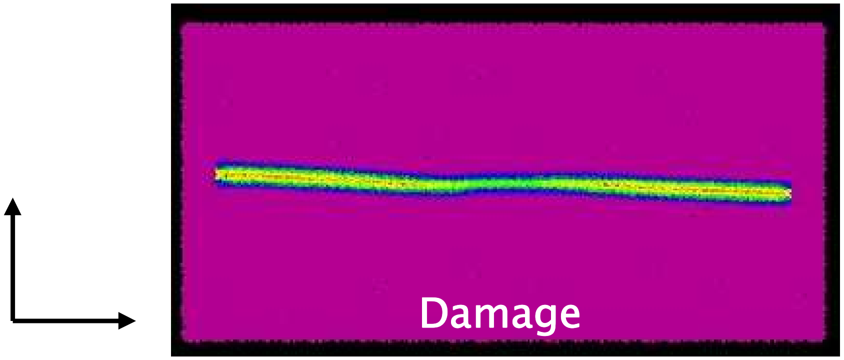
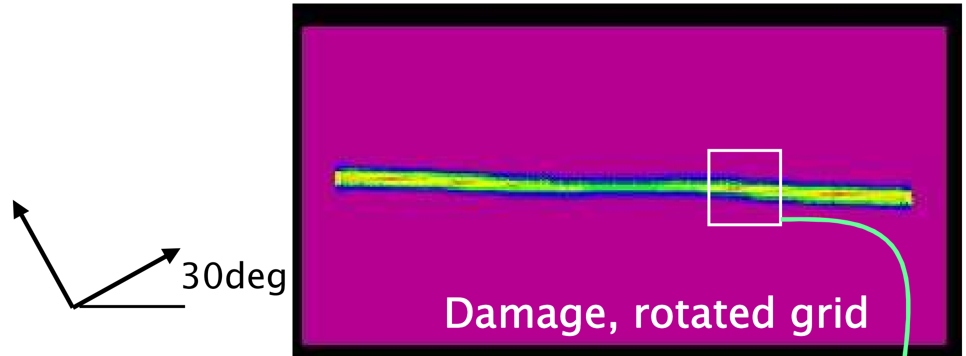
Effect of rotating the grid in the “mostly Mode-I” problem

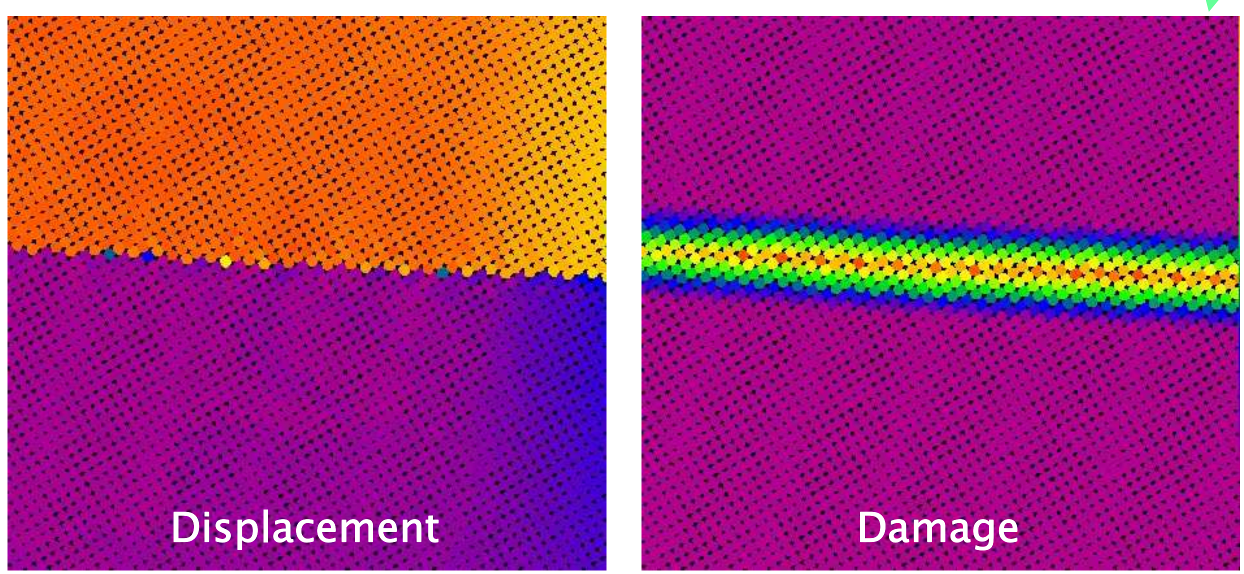


Original grid direction

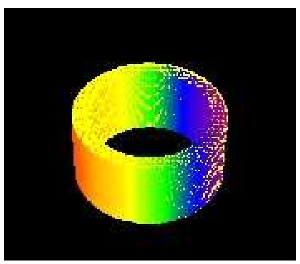


Rotated grid direction

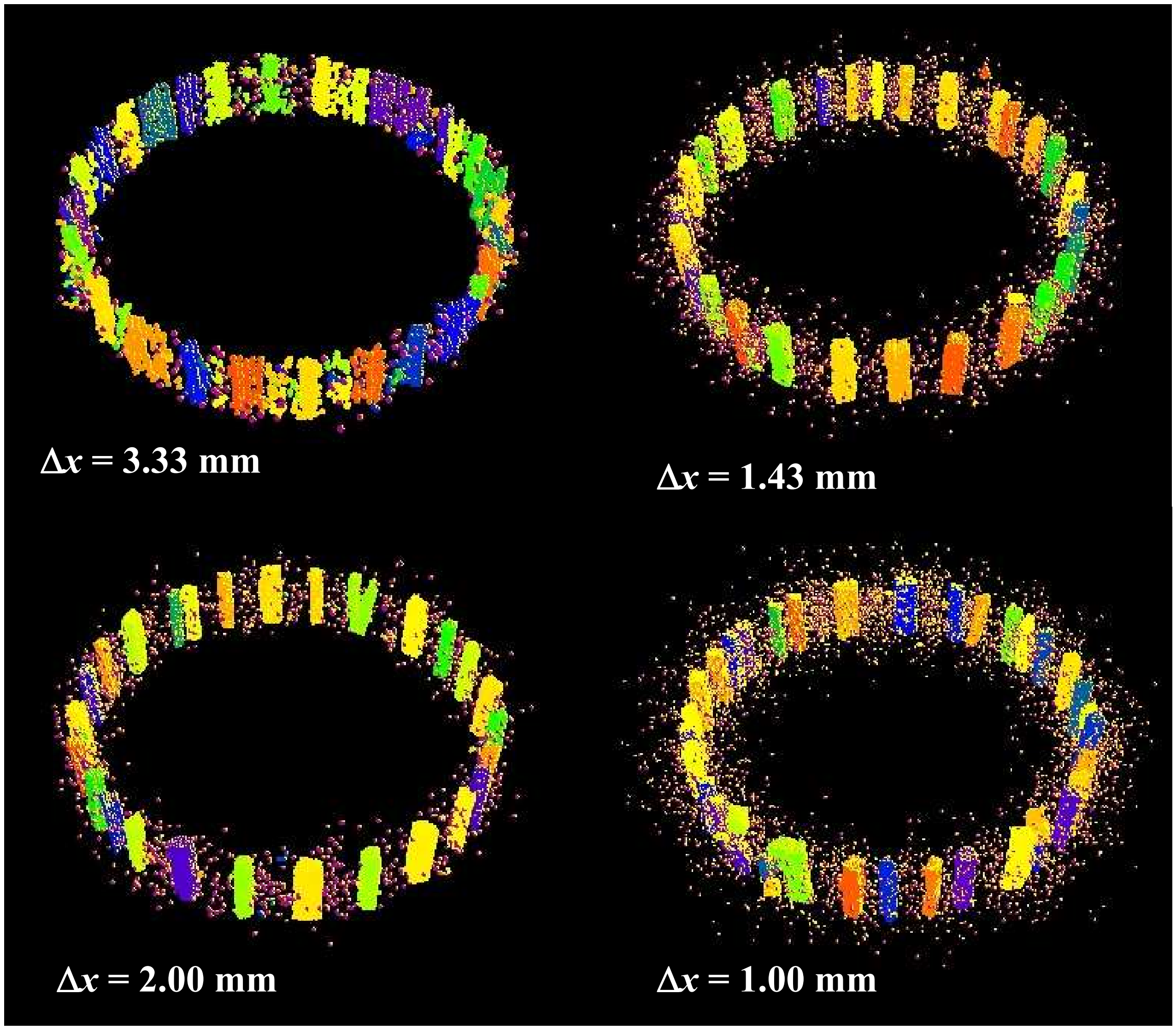
Network of identical bonds in many directions allows cracks to grow in any direction.



Fragmentation example: Same problem with 4 different grid spacings



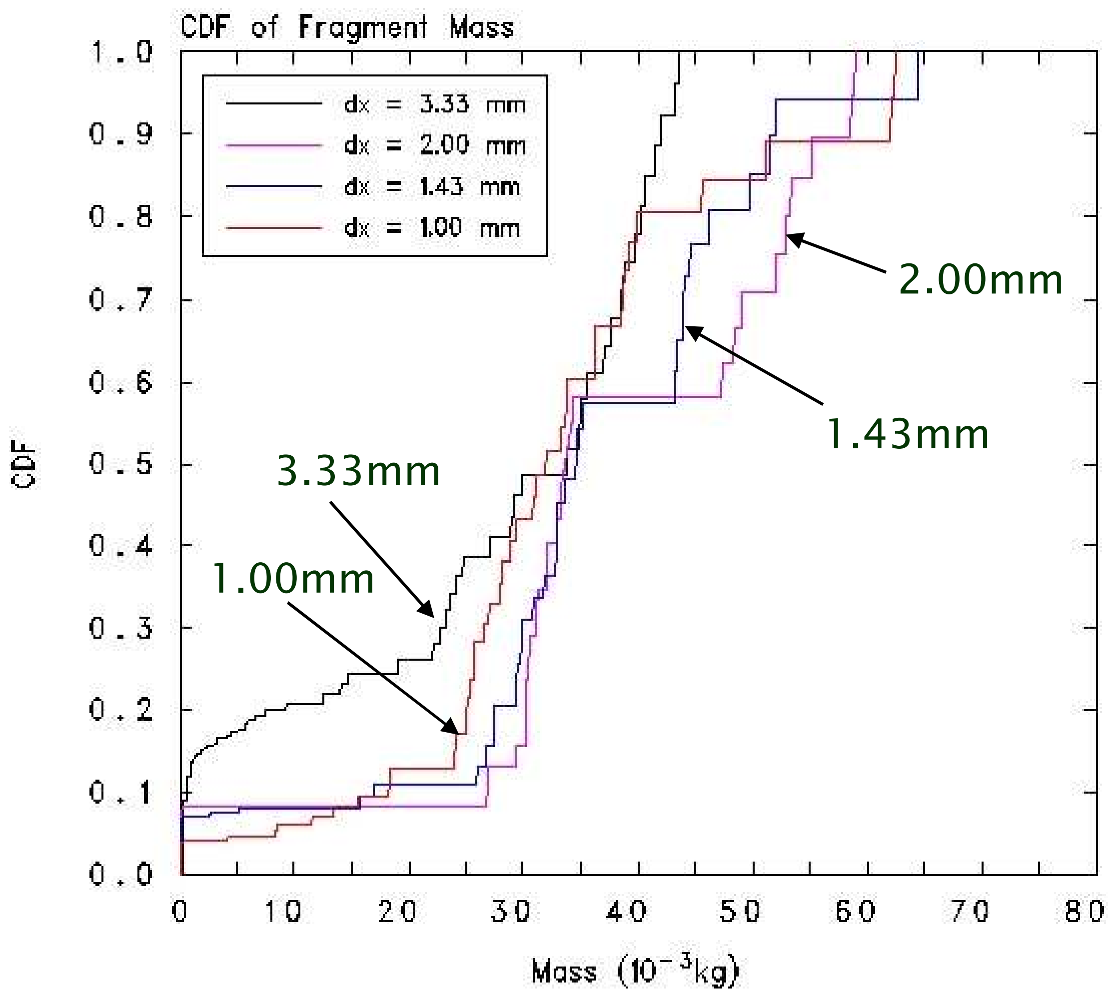
Colors are just for visualization



$$\boxed{\delta = 3\Delta x}$$

Fragmentation example: Fragment mass distribution

Cumulative distribution function for 4 grid spacings



Δx (mm)	Mean fragment mass (g)
3.33	27.1
2.00	37.8
1.43	35.9
1.00	33.5

Solution appears essentially converged

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Some current research areas

- Peridynamic theory as a coarse-graining method for atomistics.
- Dynamic crack behavior.
- Finite element solution of PD equations.
- Composite (and other) material modeling.
- Fragmentation.
- Material stability.
- Statistical mechanics foundations of PD.

Conclusions

- Peridynamic theory treats continuous and discontinuous bodies and deformations the same.
- Classical PDEs are obtained as a limiting case.
- Stress tensor is a nonlocal version of the classical PK stress.
- Mathematical consistency appears to help convergence properties of fracture simulations.